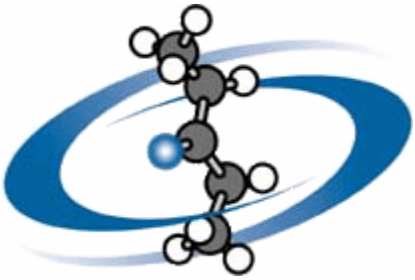

ACD/3D Viewer

Version 8.0 for Microsoft Windows

User's Guide

Viewing 3D Structures and Calculating their Structural Parameters

Advanced Chemistry Development, Inc.

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Before You Begin

Thank you for purchasing ACD/3D Viewer. We have endeavored to produce the easiest to use 3D chemical display program available today.

About This Guide

Completion of this guide should give you the tools needed to get started with ACD/3D Viewer, it is designed for either online use or to be printed and used as a “hard copy” version.

The screen shots shown throughout this reference manual have been taken with a relatively small window size.

The colors and other properties of the window elements described throughout this manual correspond with the default Windows Display Properties.

This guide is provided in electronic form, readable with Adobe Acrobat software. If you cannot locate an index topic you need please do a text string search for the relevant word or phrase, or related words.

Advanced Understanding

This guide is intended to be a part of the technical documentation for ACD/Labs software. To study ACD/Labs products gradually, we recommend the following order of working through the technical documentation:

Documents for ACD/ChemSketch and ACD/Dictionary familiarize you with features of drawing and looking up structures.

ACD/Forms Manager is required to learn how to create input dialog boxes for user data and an interface for consistent database input.

Mouse Conventions

You may perform several actions during your work with this software; the following specific words are used to describe them:

- ***Point to*** means move the mouse pointer to an item.
- ***Click*** or left-click means point to an item, and press the left mouse button.
- ***Right-click*** means point to an item, and press the right mouse button.
- ***Double-click*** means point to an item, and quickly press the left mouse button twice.
- ***Drag*** means point to an item, press and hold down the left mouse button while you move the item.
- ***Select*** means highlight or make an interface element active by either clicking it or dragging over it (other actions are possible if specified in documentation). If used in "select the check box", it means that the check box should be marked with a tick (as opposed to "clear the check box" when the check box should be cleared, without a mark).

For More Information…

To see the latest in ACD/Labs software and services, please visit our Web site at

http://www.acdlabs.com

Our Web site is being accessed at the rate of tens of thousands of “hits” per day. There’s a reason for this: much is offered through our Web site. As of Spring 2004, we offer free ChemSketch 5.0, a free ISIS 3D Add-in, free ChemDraw extensions, and a free 2-week demo key for “Interactive Laboratory” sessions where you can run test calculations using Java applets without purchasing software. There are TechSmith Camtasia-based movies which show the operation of many of our software packages (especially ChemSketch) available for download.

We are constantly updating the information on our Web site. The Web site will tell you at which scientific conferences you can visit the ACD/Labs booth. You can browse the Frequently Asked Questions page or drop in and “chat” on our newsgroup, which can also be reached via our web page.

If you would like to stay informed of the latest developments in chemical software at ACD/Labs, please be sure to sign up for e-mail broadcasts at our Web site page:

http://www.acdlabs.com/feedback/mailing.html

If you would like to partake of the ChemSketch newsgroup, please access:

news://news.acdlabs.com/acd.public.chemsketch

How to Contact Us

We are accessible through our Web site, phone, fax, and regular mail, but by far the most popular way to contact us is via electronic mail. Questions on pricing, sales, availability, and general issues should be directed to:

info@acdlabs.com

Technical and scientific support issues should be addressed by visiting:

http://support.acdlabs.com

Please tell us the name of the software purchaser; the product name, version number, build number, and license ID of the product you are contacting us about (from the **Help** menu, choose **About** to find this information); as well as a description of the problem you are having. If applicable, please tell us the name of the distributor from whom you purchased the software.

Online Updates

Version 5.0 and later of all PC-based ACD/Labs software contains the capability to have software updates delivered online. You will need the registration numbers of the software and an Internet connection from the same computer on which the software is installed. The updates are small fixes, for example, bringing the actual version number of a program from 8.00 to 8.01. For more information, refer to the "Online Updates" document included with the rest of the product documentation in your Documents folder or e-mail our technical support department.

1. Introduction

1.1 What is ACD/3D Viewer?

ACD/3D Viewer is a fast yet accurate 3D modeling and visualization program. It is fully integrated with ACD/ChemSketch, allowing you to draw 2D structures and quickly obtain their 3D representations in a striking color display. With ACD/3D Viewer you can:

- Manipulate 3D models: move, 2D and 3D rotate, resize, change styles, and colors;
- Display a 3-D structure as stick, ball-and-stick, spheres, or disks;
- Add an overlay of small-dots at approximately the van der Waals radius level to the solid 3-D structure;
- Measure and change bond lengths, plane bond angles, and torsion angles;
- Optimize the structure using a 3-D CHARMM-type of force field;
- Switch from 3D to 2D display in the ChemSketch window at the click of a button;
- Set the 3D molecule to Auto-rotate, with or without changing the style of structure display;
- View 3D structure in perspective;
- Display multiple bonds in the Wireframe view mode; and
- Export 3D models to other geometry optimization programs and use them as good starting configurations.

1.2 3D Optimization Algorithm

The 3D optimization algorithm rapidly transforms the planar (2D) structure from ChemSketch into a realistic 3-dimensional structure. It is based on modified molecular mechanics which take into account bond stretching, angle bending, internal rotation, and Van der Waals non-bonded interactions. Modifications include minor simplification of potential functions and enforcement of the minimization scheme by additional heuristic algorithms for dealing with "bad" starting conformations.

The 3D optimization algorithm is a proprietary version of molecular mechanics with the force field initially based on CHARMM parametrization.[1] The modifications involve some simplification and were intended to increase the stability and speed of computation. Note that 3D-optimizer is NOT a full-scale molecular mechanics engine. Its design aims to reliably reproduce reasonable conformations from (possibly very unreasonable) 2D drawings, rather than to precisely optimize 3D structures.

[1] Refer to B.R. Brooks, R.E. Bruccoleri, B.D. Olafson, D.J. States, S. Swaminathan, and M. Karplus. CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. *J. Comput. Chem.* 4 187–217 (1983).

Occasionally the 3D optimization produces a molecular conformation different from what you have expected. It is the very essence of the conformational analysis that molecules typically have many possible conformations. The optimizer finds only one, and it is not necessarily the one you have expected. For example, you probably expect a cyclohexane fragment to be a chair, but the optimizer may generate a twist-boat, which is also one of its suitable conformations (indeed, in many structures this fragment exists in a twisted form). To obtain another conformation, move some atoms in the resultant 3D structure to make the initial structure closer to the final conformation, and then optimize the structure once again.

If you try to obtain a specific enantiomer for a structure with chiral centers, in the process of optimization, the configuration input may occasionally change to an opposite one. To solve the problem, it is usually enough to draw all four substituents of the chiral carbon atom and use both **Up** and **Down Stereo Bond** tools to define the required direction of bonds in the initial 2D structure. If it doesn't work, you can move the atoms manually in the resulted 3D structure and optimize the structure once again. In any case, we recommend answering "No" when you are asked whether to remove hydrogens before starting optimization in the unfolding **3D Structure Optimization** dialog box.

1.2.1 Limitations of ACD/3D Optimizer

ACD/3D Viewer can only optimize structures containing atoms from Hydrogen to Xenon with standard valence and bonding states. Also, it does not take into account hydrogen bonding.

The maximum allowed number of atoms in the structure to be optimized is 250 including implicit hydrogen atoms.

2. Basics of ACD/3D Viewer

2.1 Objectives

This chapter will familiarize you with:

- Starting the program;
- Setting and changing file associations;
- Changing default directories for opening and saving files; and
- Exiting the program.

Instructions for system requirements, and for installing and uninstalling the software are provided on a separate sheet of paper, shipped with the software itself.

2.2 Starting ACD/3D Viewer

Once ACD/3D Viewer has been installed on your computer, follow these basic steps to start it:

1. Start Microsoft Windows.
2. Double-click the 3D Viewer icon.
   –OR–
   On the **Start/Run** menu in the Windows 98/2000, NT, or XP taskbar, point to **ACD/Labs**, and then choose the 3D Viewer icon.
   –OR–
   Double-click the program file SHOW3D.EXE in the folder where you have installed all ACD/Labs software. By default this is ACD8.
   –OR–
   If you have other ACD/Labs programs running, from the **ACD/Labs** menu, choose **3D Viewer**.

   You should see an opening splash screen. If this is the freeware version, you will see a 15-second list of ACD/Labs products scroll by. Be patient and click **Cancel** when it becomes active.

2.3 Setting File Associations

If this is the first time you have started the program, the **File Associations** dialog box will appear.

> **Note** If you open the **File Associations** dialog box (from the **File** menu, choose **File Associations**) under Windows NT but have no rights to change file associations, a warning message appears. Contact your system administrator to resolve this matter.

This contains a selectable list of file extensions and file types which you may want to open automatically with ACD/Labs software from now on. If so, click the check boxes of the file formats you want to add, and then click **Yes**.

If you do not want to have 3D Viewer automatically open files with the listed extension, or are not sure, leave the check boxes blank and click **No**.

2.3.1 Changing File Associations

If you have not selected all formats, the default file association can be viewed or changed at any time; from the **File** menu, choose **File Associations**. If you have selected all formats, then you receive a message, "all supported file types are already associated with the current application". In this case, you can change the file associations through Windows Explorer.

1. Open Windows Explorer, and select a file with the extension for which you want to create the association.
2. Hold down SHIFT and right-click on the file. From the pop-up menu, choose **Open With**.
3. Set the application that should be used to open the file and select the **Always use this program** check box.
4. Click **OK** and close Windows Explorer.

2.4 Changing Default Directories

If you are running a single-user (stand-alone) copy of ACD/3D Viewer, the default directory settings are likely fine.

If you have a network copy, it is advisable to change the default directory settings in the ACD/Labs software so that the default drive for saving work-in-progress is the user's local hard drive, not the remote server. After creating local access for either limited or unlimited numbers of seats, then at each local installation:

1. In the ChemSketch window, from the **Options** menu, choose **Preferences**.
2. Click on the **General** tab. In the **Default** box, specify the directory that will be opened every time you open the **Import**, **Open**, **Save**, or **Export** dialog boxes in the ChemSketch window:

> **Note** In the **Private** box you can set the directory for recording the configuration of the ChemSketch program (e.g., TEMPLATE.CFG and GRSTYLES.STL files).

3. Click **OK**.
4. Switch to the 3D window, from the **Options** menu, choose **Set Default Folder** and specify the required folder for opening and saving files. Click **OK**.

2.5 Exiting ACD/3D Viewer

You can exit from the program in any of the following ways:

- Click in the upper right-hand corner of the title bar of any window.

–OR–

- From the **ACD/Labs** menu, choose **Close All**. This will attempt to close all ACD/Labs programs that are currently open, one right after the next.

–OR–

- From the **File** menu, choose **Exit**. This will close only the currently open ACD/Labs program.

You will be prompted to save your work in the appropriate file formats, depending on the window that you are exiting.

3. Operating with Molecules View

3.1 Objectives

In this chapter you will learn how to:

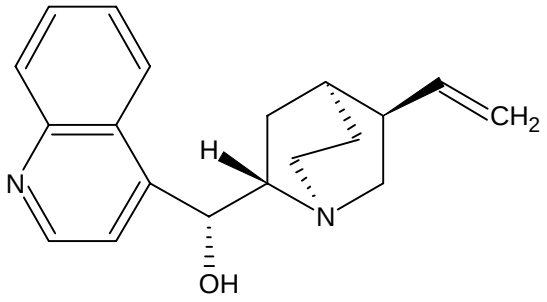
- Insert molecule into the 3D window and 3D optimize it;
- Customize the view of molecules (position, size, color, atom radii);
- Save and load view settings; and
- Measure and change the distance between atoms, and calculate and change the angle between bonds.

3.2 Inserting a Molecule and 3D Optimizing

1. Start ACD/3D Viewer as described above.
2. Click **ChemSketch** ChemSk on the Window Switching bar. This will switch you to the ChemSketch window.
3. Click **Dictionary** in the upper right part of the window.

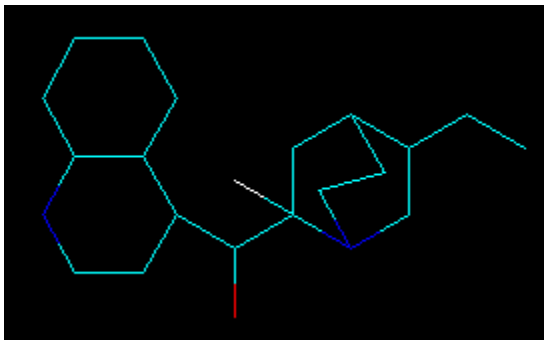
> **Note** The free ChemSketch version does not include the Dictionary module. This module is a commercial one, so if you are using a free ChemSketch program, draw any desired structure using the ChemSketch interface tools. (For details on drawing structures, refer to the *ACD/ChemSketch Tutorial*.)

4. In the **Quick Search** box of the **ACD/Dictionary** dialog box that appears, type a few keystrokes for the name "*cinchonidine*". (Cinchonidine is an anti-malarial agent that is extracted from the bark of various species of Cinchona.)
5. As soon as the required name is selected in the list and the corresponding structure is displayed, click **OK**. Note that the shadow of the selected structure hangs over the cursor. Click the workspace to place the structure in the ChemSketch window:

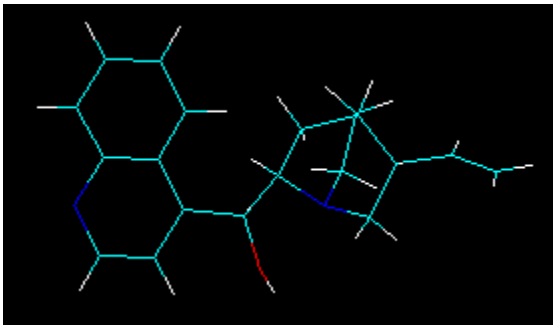


6. Click **Copy to 3D**

on the Window Switching bar to transfer the molecule into the ACD/3D Viewer interface. You will see a simple stick figure appear in the 3D window:



7. To create a 3D model of a 2D chemical structure, click **3D Optimization** . Note that the hydrogens are added:



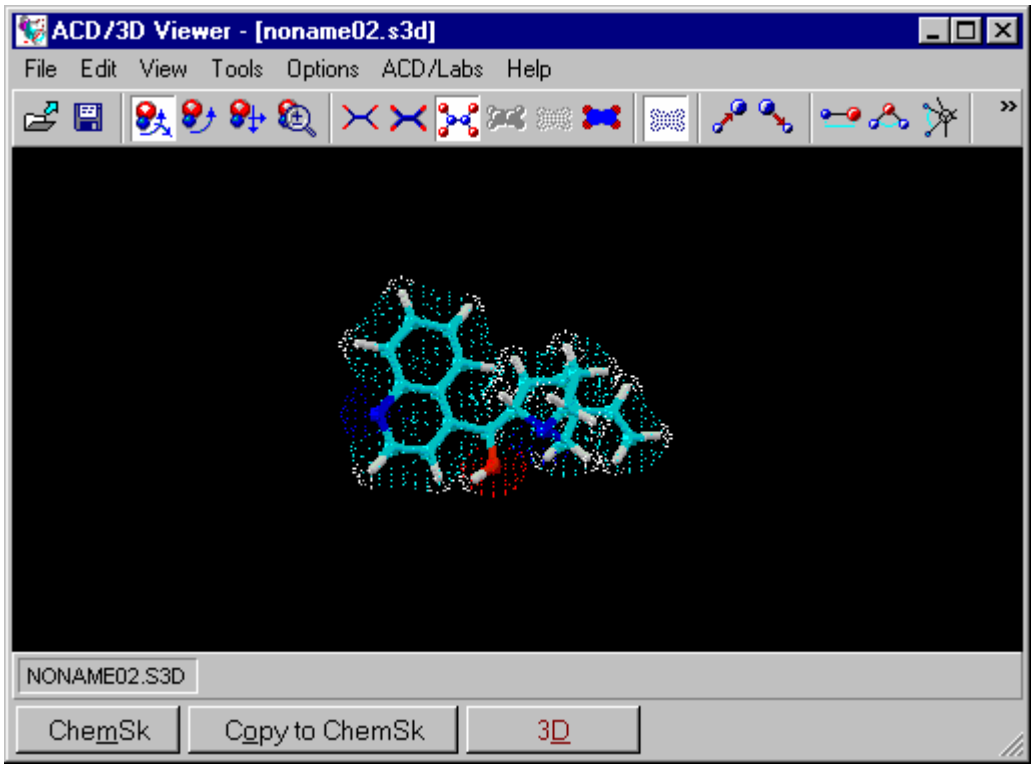
3.3 Customizing Molecule View

3.3.1 Rotating, Moving and Zooming

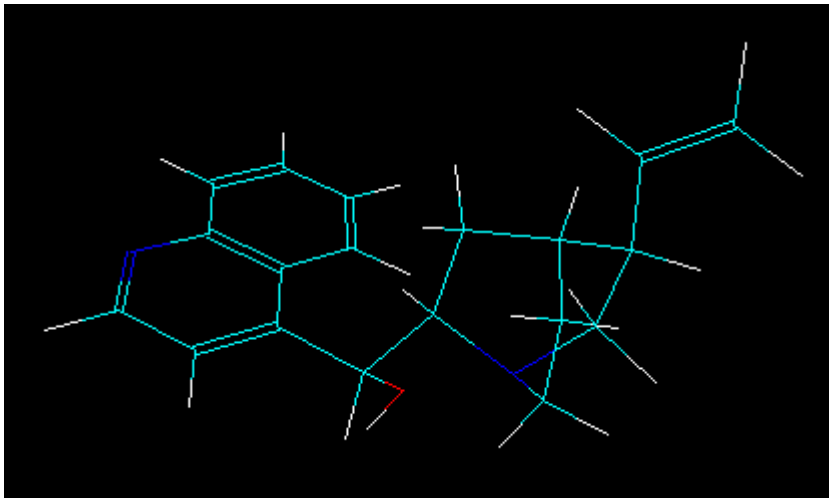
1. Click **3D Rotate** and drag over the workspace to rotate the structure in the tree-dimensional space.
2. Now switch to the Z-rotate mode by clicking **Rotate** . If you drag in the workspace now, the structure will be rotated in the two-dimensional plane only.
3. Click **Move** to enter the Drag mode where you can move the structure up, down, left, or right in the workspace.
4. To resize the structure display, click **Resize** and drag. Dragging from the center of the structure to the border of the screen makes the structure larger and dragging to the center of the structure makes it smaller.
5. Click **3D Rotate** to switch back to the 3D Rotate mode.

3.3.2 Changing Structure Representation

1. To represent the current structure as balls and sticks, click **Balls and Sticks** .
2. To add a dots halo to the current molecule view, click **With Dots** . The structure will look something like this:



3. To display multiple bonds, switch to the Wireframe mode by clicking on the Top toolbar, and then from the **View** menu, choose **Show Multiple Bonds**:

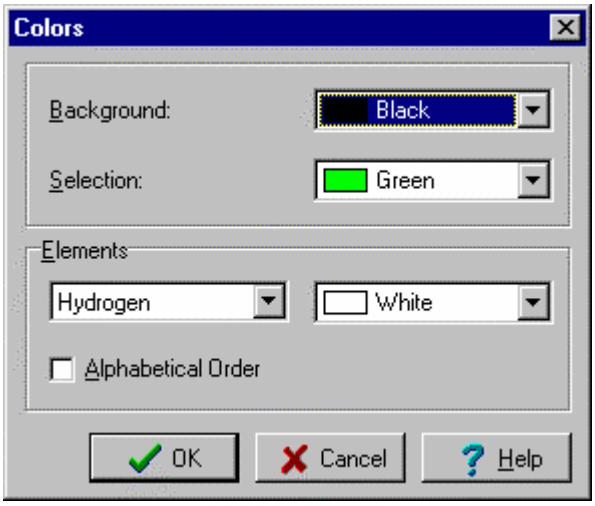


4. To rotate a molecule automatically as it is, without changing its view type, click **Auto Rotate** . (To rotate a molecule automatically, changing its view type, click **Auto Rotate and Change Style** .)

> **Note** To represent the structure as disks, wireframe, dots, or spacefilled, click the corresponding buttons on the toolbar (, , , or respectively). You can also right-click in the window workspace to switch among the view mode buttons. (Note that if any of the measure tools (, , or) are active, right-clicking will toggle between them only.)

3.3.3 Changing Colors

1. From the **Options** menu, choose **Colors** or click **Set Colors** to display the **Colors** dialog box:



2. To change the color of the background of the display, select the desired color in the **Background** list.

> **Tip** If you are printing a lot, it is best to change the background to white to save toner.

3. When measurements are being made, the set of atoms whose distance or angles are being measured are given a special highlight color. The default is bright green. To change the color of the atoms that are selected, from the **Selection** list, choose the desired color and click **OK**.

> **Note** Selection works only with the **Distance** , **Angle** , and **Torsion Angle** tools.

4. To change the color of a chemical element, click the name of the element in the list and then choose the desired color to the right.

> **Note** Selecting the **Alphabetical Order** check box sorts the names of the elements in the list; otherwise, the elements are listed in the order they appear in the Periodic Table of Elements.

3.3.4 Obtaining the Mirror View

1. Click **Mirror** to obtain a mirror image of the currently displayed structure. All the stereo centers present in the initial structure will be inverted in this case.
2. To return back to the initial view, click this button again.

3.3.5 Inverting Structure Center

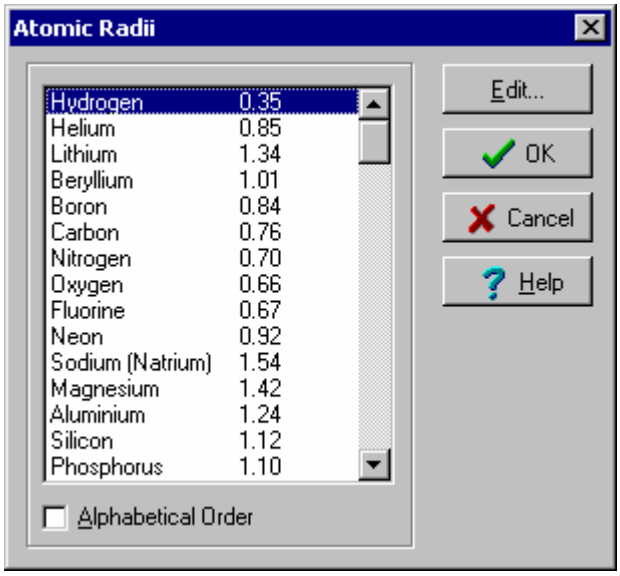
1. Click **Invert Center** , and then click the atom to invert. This tool inverts the configuration of chiral center by changing the spatial position of one or several substituents of the selected atom.

   > **Note** After the current operation it may be necessary to optimize the chemical structure once more. To perform this, click **3D Optimization** on the Top toolbar.

2. To return back to the initial structure view, click **Invert Center** again.

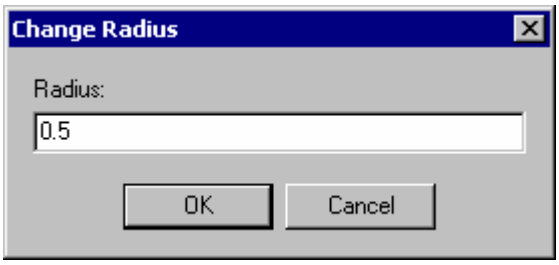
3.3.6 Changing Atom Radius of a Specific Element

1. From the **Options** menu, choose **Radii** to open the **Atomic Radii** dialog box containing the default settings for atom radii of various elements:



2. To view the currently set radius of any element, click it in the list. In the right column the corresponding value is highlighted.

3. To change the atom radius for an element, double-click it in the list and type the new value, e.g., *0.5*, in the **Change Radius** box that appears:



4. Click **OK** to save changes.

> **Note** The atomic radius is expressed in relative units.

5. As soon as the changes are made in the **Atomic Radii** dialog box, click **OK**. Next time you start ACD/3D Viewer, the default values will be reset to their previous values. For more details on how to save and load default settings, refer to Section 3.4.

3.3.7 Changing the Display of Atom Radius

1. Click **Increase Atoms' Radii by 5%** . Each additional click on this button increases the radii of all displayed atoms by 5%.
2. Click **Decrease Atoms' Radii by 5%** to decrease the radii of all displayed atoms by 5%.

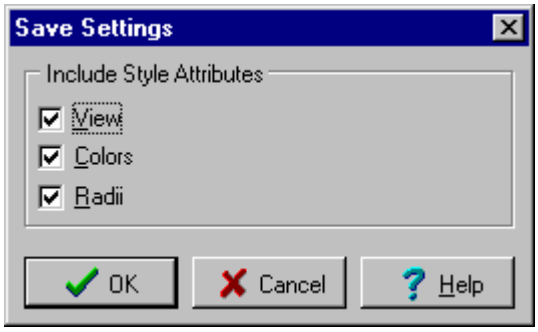
> **Important** These tools do not affect the actual radii of atoms (those specified in the **Atomic Radii** dialog box), but only change the display.

3.4 Saving and Loading View Settings

You can save settings that you have specified during the current work session as a .3DS file, load them from a previously saved file, and set them as the new default.

3.4.1 Saving View Settings

1. From the **Options** menu, choose **Save Settings** to display the following dialog box.



2. Select the check boxes of the attributes that you want to be saved. Note that selecting the **Radii** check box will allow you to save settings specified in the **Atomic Radii** dialog box, but not the current radius display options (see Sections 3.3.6 and 3.3.7).

3. Click **OK** and in the dialog box that appears, specify the name of the file and location (drive and directory). Note that the file should be saved with a .3DS extension.
4. Click **Save** to save the file.

3.4.2 Loading View Settings

If you have previously saved the view settings, you can load them for the current session.

1. From the **Options** menu, choose **Load Settings** to open the **Load Settings** dialog box.
2. Find the .3DS file you want to load.
3. Click **Open**. The settings contained in this file will be loaded for the current working session.

3.4.3 Setting Default View Settings

If you want to use specific settings each time you work with ACD/3D Viewer, you should set them as default ones.

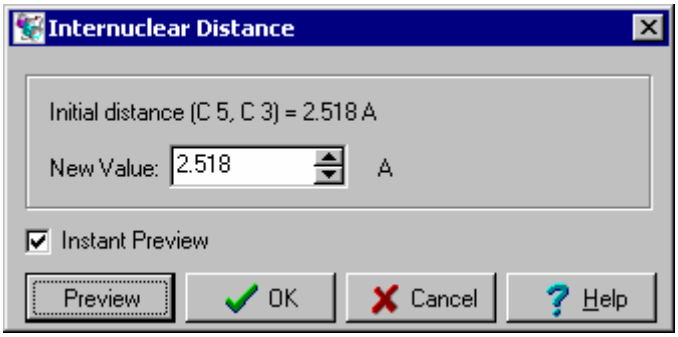
1. Specify the required view settings (refer to Section 3.3).
2. To save them to a file, from the **Options** menu, choose **Save Settings**.
3. From the **Options** menu, choose **Set Default Settings** to open the **Set Default Settings** dialog box.
4. Find the file with the setting you want to set as the default.
5. Click **Open**. From this point on, each time you open ACD/3D Viewer these settings will be loaded until you specify other ones.

> **Tip** To return to the system default settings, from the **Options** menu, choose **Restore Default Settings**.

3.5 Calculating and Modifying Structural Parameters

3.5.1 Calculating and Changing Distance Between Two Atoms

1. Switch to the **Balls and Sticks** view mode ( ) for a better view of the atoms.
2. Click **Distance** .
3. Click any atom to select it, and then move the mouse pointer over another atom to highlight them with the selection color. The **Internuclear Distance** dialog box appears:

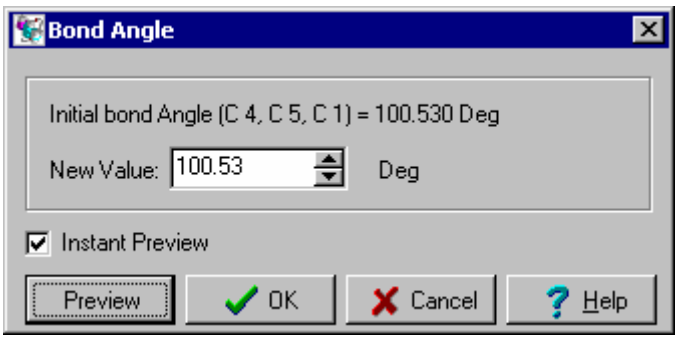


Also, on the status bar you can see the distance between the selected atoms:

4. To change the distance, in the **Internuclear Distance** dialog box, type the desired value in the **New Value** box. If the **Instant Preview** check box is selected, the changes are immediately applied. If the check box is not selected, after each change you need to click **Preview**. The initial distance is always present in the dialog box, so if you decide not to change the distance, you can easily return to the initial settings.
5. Click **OK** to apply changes (if any) and close the dialog box.
6. To cancel the selection and to start a new measurement, click somewhere in the empty workspace. To stop using this tool, click on its button to deselect it.

3.5.2 Calculating and Changing the Angle Between Two Bonds

1. Click **Angle** .
2. Click two neighboring atoms which form a bond.
3. Move the mouse pointer to the third atom which makes a bond with the last selected one. The **Bond Angle** dialog box appears:

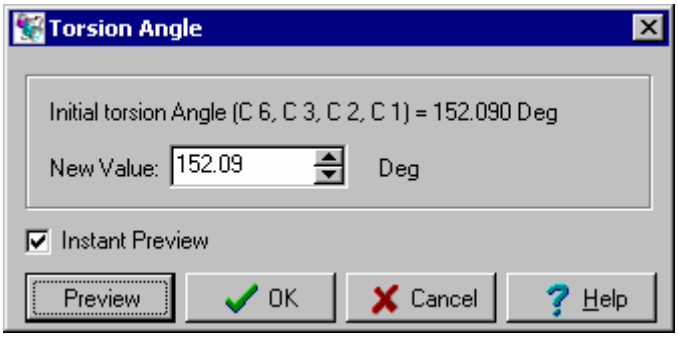


Also, the calculated angle value appears on the status bar, for example,

4. To change the angle, in the **Bond Angle** dialog box, type the desired value in the **New Value** box. If the **Instant Preview** check box is selected, the changes are immediately applied. The initial angle is always present in the dialog box, so if you decide not to change the angle, you can easily return to the initial settings.
5. Click **OK** to apply changes (if any) and close the dialog box.
6. To cancel the selection and start a new measurement, click somewhere in the empty workspace. To stop using this tool, click on its button to deselect it.

3.5.3 Calculating and Changing a Torsion Angle

1. Click **Torsion Angle** .
2. Click two atoms participating in a common bond. The corresponding bond becomes selected.
3. In the same manner, click two more atoms adjacent to a previously selected bond. The final result will be three adjacent bonds, participating in a torsion angle, which will be selected. The **Torsion Angle** dialog box appears:



> **Note** Without selecting the third bond, it is possible to look through the values of all possible torsion angles neighboring the last selected atom by moving the mouse pointer over adjacent atoms.

4. Try changing the value in the **New Value** box. If the **Instant Preview** check box is selected, the changes are immediately applied. The initial torsion angle is always present in the dialog box, so if you decide not to change the angle, you can easily return to the initial settings.
5. Click **OK** to apply changes (if any) and close the dialog box.
6. To cancel the selection and to start a new measurement, click somewhere in the empty workspace. To stop using this tool, click on its button to deselect it.

4. Creating an Animated GIF

With help of ACD/3D Viewer you can create animated .GIF files for your site with minimum effort, minimum cost, and maximum impact.

The GIF file format may not be as sophisticated as Java, Flash, ActiveX, or more chemistry-oriented formats such as RasMol and Chime, but these newer applications are not as accessible to casual Web visitors who may not have the appropriate plug-ins or a connection that is fast enough. For true accessibility, a .GIF file is still the cornerstone of Web design.

Animated GIFs are a nice touch for many Web pages, whether to emphasize something on the page (e.g., the "New" revolving spheres on the ACD/Labs download page) or to show, pictorially, something which is better sketched while explaining it to someone (e.g., electron density movement in the course of a Diels-Alder reaction).

4.1 Obtaining the Animation Software

Animated GIFs can be created with commonly available software such as packages listed through the Tucows site.[2] Such software is often freeware, evaluation ware, or shareware. (Disclaimer: ACD/Labs makes no recommendation or claim for one animation product over another.) For the present example, we used Animagic shareware from RTL Software, Inc. An evaluation or shareware copy can be downloaded from the Web page

http://www.rtlsoft.com/animagic

and installed on your PC.

An animated .GIF file can be created by linking, in succession, one "still" or “snapshot” GIF image after another. Each still GIF contains *nearly* the same image as the previous GIF, but is changed just enough to give the human eye the illusion of movement when one GIF is shown after the other. Good animation software will optimize the linkage so that the size of the overall animated GIF will be as small as possible.

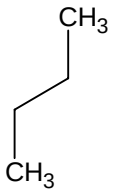
The export of a ChemSketch or 3D file to GIF format is straightforward. A set of these GIFs is used as input to a special GIF-animator program, which will output the moving image (after some editing and optimization) to the animated GIF format. We go through these steps in detail below.

[2] TUCOWS is an acronym for The Ultimate Collection of Windows Software. See www.tucows.com.

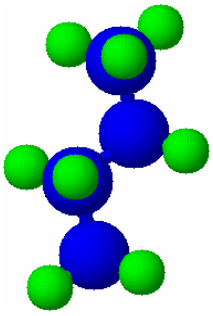
4.2 Step-Wise Motion in ACD/3D Viewer

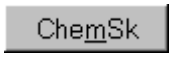
We will start with a very simple structure—butane—that is easy to draw and process.

1. In the ChemSketch window, Structure mode, draw butane:



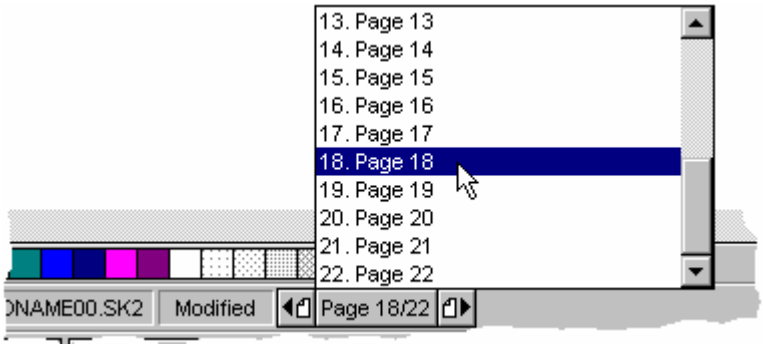
2. Click **Copy to 3D** on the Window Switching bar.
3. In the 3D window, click **3D Optimization** to optimize the structure.
4. Switch to the **Balls and Sticks** view ( ) and click **Increase Atom's Radii** several times to make the atoms more prominent.
5. From the **Options** menu, choose **Colors** and in the **Element** section of the dialog box, set the green color for hydrogen and blue color for carbon. In the **Background** section, choose **White**. You should obtain something like the following:



6. Now copy the molecule to the Clipboard; from the **Edit** menu, choose **Copy**.
7. Switch to the ChemSketch window by clicking **ChemSketch**  on the Window Switching bar.
8. If there is anything drawn in the current page, create a new page by clicking .
9. Press CTRL+V to make a fast paste of the image from the Clipboard. Click in the workspace to place the image.
10. Switch back to the 3D window by clicking **3D** , make sure that the 3D Rotate mode is on and slightly rotate the structure by dragging over it.
11. Again, copy the structure to the clipboard, switch to the ChemSketch window, create a new page, and paste the structure.
12. Repeat the steps above until your structure appears in the same position as it was at the first step.

> **Tip** To make structure rotate strictly horizontally and evenly, drag the cursor strictly horizontally and to the same destination each time.

13. Switch to the ChemSketch window. As a result of repeated pastes to new pages you should have a document with a series of pages each containing a "snapshot" of the rotating molecule. You may check the number of pages and switch between them by clicking **Page** on the status bar:



4.3 Fine-tuning the Pictures

If you look through all the pictures, you will notice that the size of each picture is different. This will affect the final animation and will make it uneven. If your animation software allows you to change the size of the used gifs and modify their contents, you can skip this section and do the necessary changes in your animation software. If you are using animation software that does not include these capabilities, you can use the Draw mode in ACD/ChemSketch to help standardize the image of each snapshot.

1. Display the page with the biggest picture on it.
2. In the Draw mode, choose the **Rectangle** tool and drag over the picture of the molecule so that the rectangle fully includes the molecule. Release the mouse button to fix the rectangle and click **Send to Back** to send the rectangle to the background so that the molecule is visible.
3. Press CTRL+A to select both objects, click **Center Horizontally** and then **Center Vertically** to align the objects relative each other.
4. If you do not want the border of the rectangle to be visible, select the rectangle only, and then right-click the left-most crossed section on the Color Palette (above the status bar) to set the border's color to **None**. Left-clicking any color will change the fill color of the rectangle—this can be useful if you have used any special background color when copying molecules in the 3D window.

   > **Note** If there is no Color Palette displayed, refer to the **View** section of the **General** tab in the **Preferences** dialog box (**Options** menu). The **Palette** check box should be selected.

5. As soon as the rectangle is of the desired color and size, select it alone and copy it to the clipboard so that you can then simply paste it for other snapshots.
6. Switch to the next page, press CTRL+V and click the molecule to paste the rectangle over it. Then click **Send to Back**, press CTRL+A to select both objects and align them by clicking **Center Horizontally** and **Center Vertically**.
7. Repeat step 6 for each page.

4.4 Obtaining a Series of GIFs

1. From the ChemSketch page list, scroll to the first 3D image (likely page 1 or 2).

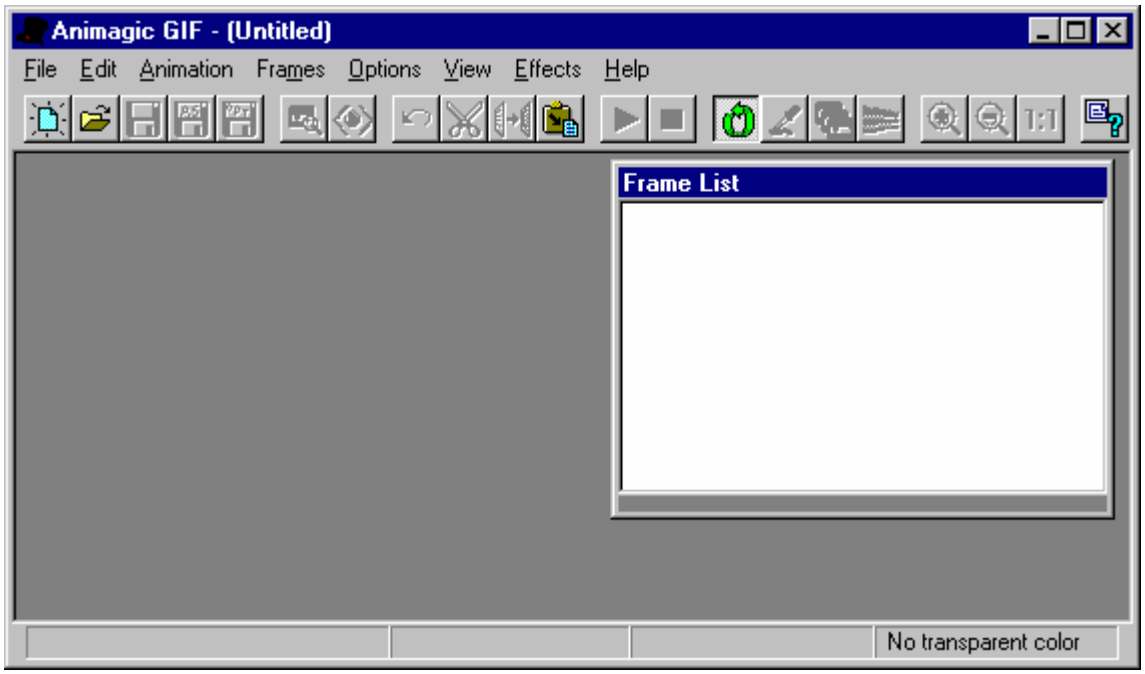
   > **Important** When exporting to a .GIF file, ChemSketch exports the whole page with no regard to whether the objects are selected or not, so make sure that the page contains only those objects that you want to appear in a .GIF file.

2. From the **File** menu, choose **Export**, and select **GIF Bitmaps (.GIF)** as the format to be saved in. Specify the name for the file, e.g., BUTANE01.GIF.
3. Click **OK** and the image on that page will be saved.
4. Move to the next page by clicking **Next Page** on the status bar or PAGE DOWN on your keyboard.
5. Repeat steps above, saving the files under a slightly different name each time in the sequence BUTANE02.GIF, BUTANE03.GIF, BUTANE04.GIF, *etc*.

4.5 Final Stage: Animating

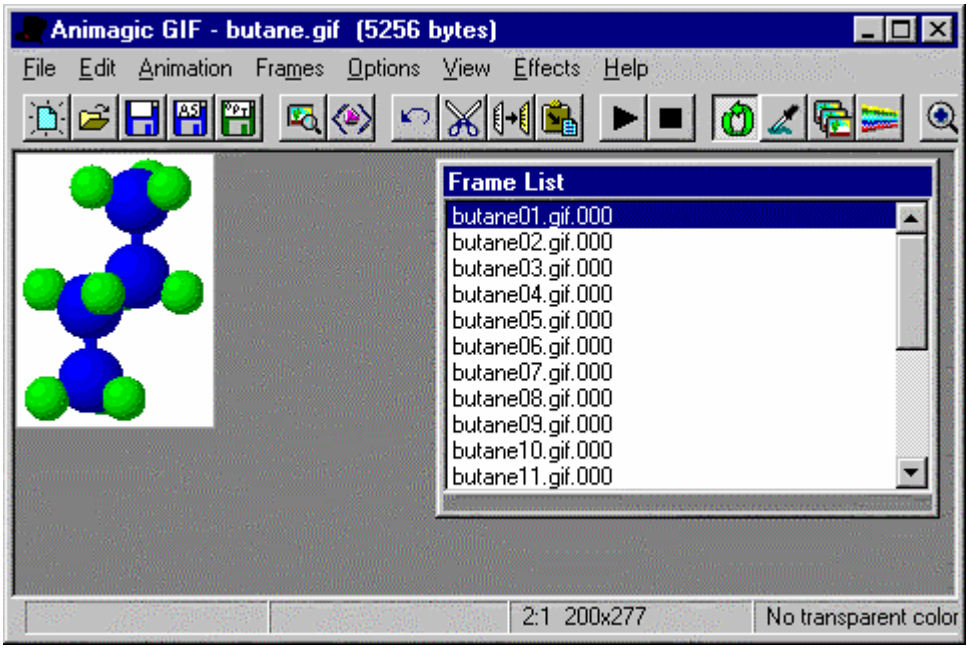
Depending on the animation software, the interface for input of .GIF files differs. The following is described with respect to the Animagic software package from RTL Software.[3]

1. Open the animation software.



[3] This is not intended as a product endorsement.

2. Insert the series of BUTANE0*.GIF files as frames into the frame list. For example, in Animagic it can be done with a drag-and-drop operation. Make a multiple selection of the file icons from their folder (or from Windows Explorer) and drag them until they are in the **Frame List** panel:



3. Click **Play** to step through the animation frame by frame.
4. Click **Loop** to make the movement repeat endlessly.
5. Add or remove GIFs as needed to complete the motion smoothly.
6. You may wish to explore other options such as setting color scales, time dwells, dirty rectangles, *etc.* in order to enhance the animation or make a smaller .GIF file.
7. From the **File** menu, choose **Save Optimized As,** and then enter BUTANE.GIF.
8. Open this file in your Web browser to view it. You can open it by drag and drop or by entering the file path as an URL.